

What is claimed is:

Claims

1. A method for use in deriving fixed bond information, comprising:
analyzing a delocalized representation of a chemical structure;
determining, based on a table of electronic state and valence distributions,
electronic and bonding characteristics for at least one atom in the chemical
structure; and
producing, based the electronic and bonding characteristics, a fixed bond
representation of the chemical structure.
2. A system for use in deriving fixed bond information, comprising:
an analyzer analyzing a delocalized representation of a chemical structure;
a determiner determining, based on a table of electronic state and valence
distributions, electronic and bonding characteristics for at least one atom in the
chemical structure; and
a producer producing, based the electronic and bonding characteristics, a
fixed bond representation of the chemical structure.
3. Computer software, residing on a computer-readable storage medium,
comprising a set of instructions for use in a computer system to help cause the
computer system to derive fixed bond information, the instructions causing the
system to:
analyze a delocalized representation of a chemical structure;

determine, based on a table of electronic state and valence distributions,
electronic and bonding characteristics for at least one atom in the chemical
structure; and

produce, based the electronic and bonding characteristics, a fixed bond
representation of the chemical structure.

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